# FINAL REPORT

## COMPUTER PROGRAM FOR THE NUMERICAL TREATMENT OF THEMODYNAMIC DATA FOR ARSENIC BASED SYSTEMS

**prepared for:**

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CDT
Centre de Développement Technologique
École Polytechnique de Montréal

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# COMPUTER PROGRAM FOR THE NUMERICAL TREATMENT OF THERMODYNAMIC DATA FOR ARSENIC BASED SYSTEMS

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**by:**

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## INTRODUCTION

Arsenic, As, is an undesirable toxic element in the production of Cu, Ni and Co metals. Its presence in high concentrations can prevent the treatment of certain ores. Research into testing and developing effective processes for removing As requires, among other things, good thermodynamic data on the various metal arsenates. Unlike the case for sulphur bearing compounds, there are limited reliable data on As compounds.

Currently, the thermodynamic properties of selected systems are being studied at CANMET by the use of an oxygen probe. For example, the partial pressure of oxygen in equilibrium with an NiAs - NiO mixture in a known partial pressure of $As_4O_6$ as defined by the following equilibria

$$NiAs(s) + 1.25O_2(g) = NiO(s) + 0.25As_4O_6(g) \qquad \text{Eq (1)}$$

can be measured by means of an oxygen probe.

In order to deduce, from the experimental results, an expression for the standard Gibbs energy of formation of NiAs, it is necessary to have:

(i) analytical expressions as a function of temperature for the Gibbs energy of formation of the other species (i.e. NiO, $O_2$ and $As_4O_6$);

(ii) a computer algorithm that first accepts as input the analytical expressions found in (i) as well as the measured oxygen probe emf, temperature, etc., and then applies a regression analys in order to calculate the expression for the measured standard Gibbs of formation of NiAs(s).

COMPUTER PROGRAM

A computer program called FORT.ARSENIC (hereafter called FORT) has been written and is listed in Annexe A. FORT reads data that have been entered by the user and stored in DATA.ARSENIC (hereafter called DATA). A simplified set of data (supplied by CANMET) are found in Annexe B and correspond to initial measurements made on NiAS-NiO mixtures represented by equation (1). These data are used only for purposes of describing the computer program and do not represent the final measurements for this system.

With reference to Annexe A (FORT) and Annexe B (DATA), FORT initially reads from DATA a general description of the experiment (2nd RUN NOV. 3). This is followed a description and known thermodynamic data for each compound in the chemical reaction (equation (1)).

There are 3 lines of data per compound:

1st line: a description of the phase (O2(g))
2nd line: the stoichiometric factor in the equation with negative values for reactives and positive values for products (- 1.25)
3rd line: DH(298), S(298) and the coefficients A, B, C and D of the heat capacity expression CP = A + B.T + C/T**2 + D.T **2

The data for the 3rd line could be taken from the F*A*C*T system (Annexe C) or supplied by the user. Note all units are in calories.

The arsenic bearing phase which is being measured (NiAs) is entered last but the 3rd line is left blank.

All the data that have been entered to this point are only used AFTER the least squares analysis of the experimental measurements. It is not necessary to enter them and they may be replaced by a blank line representing the 1st line of the 1st phase (02).

Experimental data are entered next. Each experimental point consists of 4 values and these are entered on one line:

(1) temperature (K)
(2) measured EMF (mV)
(3) reference oxygen potential (atm) and
(4) arsenolite bath temperature (K).

Entry is terminated by a blank line.

The data are then treated in a least squares algorithm (subroutine SQUARE) from which is calculated the expression for the standard Gibbs energy change of the reaction (equation 1) represented first as a 2 and then as a 3 coefficient equation as shown in Annexe D.

This is followed by a table that contains for each data point:

DGZERO - measured Gibbe energy change
DGCALC - calculated value using the 2 or 3 coefficients
DG(DEVN) - difference between experimental and calculated values of the Gibbs energy change
EMF - measured emf
EMFCALC - calculated emf

EMF(DEVN) - difference between the measured and calculated emf
TK - cell temperature (kelvin)
PO2REF - the cell reference potential (atm)
O2(EXP) - the experimentally measured oxygen potential (atm)
BATHTK - the arsenolite bath temperature (kelvin)
PAS406 - the partial pressure of As406(g) calculated from the following expression taken from Behrens and Rosenblatt (J. Chem. Therm., Vol. 4, p. 175, 1972):

$$\log 10 \text{ (PAS406 atm)} = -6067/T + 9.905 \qquad \text{Eq (2)}$$

The relationships between EMF, TK, PAS404, etc. are given at the top of FORT.ARSENIC (Annexe A).

Following the table are printed DH(298), S(298), A, B, C and D of the unknown arsenic bearing compound. These values are calculated only if thermodynamic data were entered for the other compounds in the reaction (equation 1) prior to entry of the experimental results.

## ANNEXE A - Listing of the computer program FORT.ARSENIC

```
/SYS REGION=MAX
/LOAD WATS
/OPT INFO
C    *** O2-ARSENIC EMF TREATMENT ***
       IMPLICIT REAL*8(A-H,O-Z)
       REAL*4 SXX(72)
      COMMON/LANGUE/LANG
       COMMON/COM1/$PHASE(10,18),DH298(10),S298(10),CPA(10),CPB(10)
      1,CPC(10),CPD(10),GA(10),GB(10),GC(10),GD(10),GE(10),GF(10)
      2,GG(10),STOIC(10),M1
       DIMENSION TK(99),EMF(99),PO2(99),AK(99),
      1 DGZERO(99),X(99,3),$TITRE(18),Q(3)
      2,PO2REF(99),BATHTK(99)
       DATA $BLANK/' '/
C-------------------------------------------------------------------------
C
C   CP = CPA + CPB*TK + CPC/TK*TK + CPD*TK**2
C
C
C CHEMICAL REACTION:
C
C   Metal-arsenate(s) = Metal-oxide(s) + I.O2(g) + J.As4O6(g)
C
C CELL EMF:
C
C    E = (RT/4F)*Ln(PO2/PO2REF)
C
C i.e.,   PO2 = PO2REF*exp(E*4F/RT)
C
C   DGZERO = -R.T.Ln <AK>
C
C          = -R.T.Ln <P(O2)**I . P(As4O6)**J>
C
C          = a + b.TK + c.TK.log10(TK)
C
C   HENCE
C
C        EMF =  (DGZERO + R.T.ln<PO2REF**I> + R.T.ln<PAS4O6**J>)/(-4FI)
C
C
C VARIABLES:
C
C    TK       cell temperature in kelvin                    ;
C    DH298    standard enthalpy of formation at 298K        ;
C    S298     absolute entropy at 298K                      ; see INSPECT
C    CPA      heat capacity coefficient                     ; (F*A*C*I)
C    CPB                 "                                  ;
C    CPC                 "                                  ;
C    CPD                 "                                  ;
C    GA-GG    free energy variables used in the calculation
C    EMF      emf in mv
C    PO2      oxygen pressure in atm.
C    AK       equilibrium constant K
C    SXX      dummy variable
C    DGZERO   standard Gibbs energy change
C    X        regression matrix
C    $TITRE   description of data
C    Q        computed coefficients a, b and c
C    PO2REF   reference oxygen pressure in atm.
C    BATHTK   bath temperature in kelvin
C    PAS2O6   vapour pressure of As4O6 (atm) in the bath calculated
C             from the data of Behrens & Rosenblatt, J.Chem. Therm. 1972
C    FARAD    Faraday's constant
C    RGAS     gas constant (calories)
C    FACTO    value of I in the reaction
C    FACTAS   value of J in the reaction
C-------------------------------------------------------------------------
```

```
C
C     INITIATE THE CONSTANTS
C
      PAS406(T)=10.0**(-6067./T + 9.905)
      LANG=1
      FARAD=23.065
      NR=5
      NW=6
      RGAS=1.987D00
C
CCC   DESCRIPTION OF THE SYSTEM
CC    1 line ------------------------------->
C
        READ(NR,20,END=999)($TITRE(J),J=1,18)
        WRITE(NW,30)($TITRE(J),J=1,18)
C
CCC   ENTRY OF KNOWN DH298, S298, AND CP DATA - OPTIONAL ^
CCC
CCC   Enter 3 lines per phase  ------------->
CCC   1st line: $PHASE
CCC   2nd line: STOIC (negative values for reactives, fractions accepted)
CCC   3rd line: (1) DH298 (2) S298 (3) CPA (4) CPB (5) CPC and (6) CPD
CCC   For the case of the unknown phase, enter it last of all and
CCC   leave the 3rd line blank (or the value 0).
C
        M=0
1       M=M+1
        M1=M-1
        READ(NR,20,END=999)($PHASE(M,J),J=1,18)
        IF($PHASE(1,1).EQ.$BLANK)GO TO 3
        CALL READER(SXX,NR,1)
        STOIC(M)=SXX(1)
        CALL READER(SXX,NR,6)
        DH298(M)=SXX(1)
        S298(M)=SXX(2)
        CPA(M)=SXX(3)
        CPB(M)=SXX(4)
        CPC(M)=SXX(5)
        CPD(M)=SXX(6)
        IF(SXX(1).NE.0.0.OR.SXX(2).NE.0.0.OR.SXX(3).NE.0.0)GO TO 1
3       CONTINUE
        IF(M1.GT.0)CALL GFUNC
        IF(M1.GT.0)WRITE(6,80)(($PHASE(I,J),J=1,18),STOIC(I),DH298(I),
       *S298(I),CPA(I),CPB(I),CPC(I),CPD(I),I=1,M1)
        WRITE(NW,950)
C
CC    STOICHIOMETRIC FACTORS I AND J:
CC    (Negative values for reactives, fractions accepted)
CC    COMPOUNDS(S) = COMPOUND(S) + I.O2(G) + J.AS406(G)
C     1 line ------------------------------->
        CALL READER(SXX,NR,2)
        FACTO=SXX(1)
        FACTAS=SXX(2)
        WRITE(NW,35)FACTO,FACTAS
C
CCC   EXPERIMENTAL VALUES: (1 SET PER LINE, END WITH BLANK LINE)
C     1-TK  2-EMF(MV)  3-P(O2) REF.  4-ARSENILITE BATH TK
C     one set of data per line ------------->
        I=0
15      CALL READER(SXX,NR,4)
           IF(SXX(1).LT.1.0)GO TO 50
           I=I+1
           TK(I)=SXX(1)
           EMF(I)=SXX(2)
           PO2REF(I)=SXX(3)
           BATHTK(I)=SXX(4)
           X(I,1)=1.0D00
           X(I,2)=TK(I)
           X(I,3)=TK(I)*DLOG10(TK(I))
           PO2(I)=PO2REF(I)*DEXP(EMF(I)*4.0D00*FARAD/(RGAS*TK(I)))
           DGZERO(I)=-RGAS*TK(I)*DLOG(PO2(I)**FACTO
     1                    *PAS406(BATHTK(I))**FACTAS)
        GO TO 15
50      N=I
```

```
C   LEAST SQUARES ANALYSIS
C
      DO 100 MM=2,3
         Q(3)=0.0D00
         CALL SQUARE(DGZERO,X,N,N,MM,Q,DSUM)
         RMS=(DSUM/FLOAT(N))**(0.5)
         WRITE(NW,70)Q(1),Q(2),Q(3),RMS
         WRITE(NW,71)
         DO 200 I=1,N
            DGCALC=Q(1)+Q(2)*TK(I)+Q(3)*TK(I)*DLOG10(TK(I))
            DGDEVN=DGZERO(I)-DGCALC
            AK1=DEXP(-DGCALC/(RGAS*TK(I)))
            EMFCAL=(DGCALC+RGAS*TK(I)*DLOG(PAS406(BATHTK(I))**FACTAS)
     *      +DLOG(PO2REF(I)**FACTO))/(-4*FARAD*FACTO)
            EMFDEV=EMF(I)-EMFCAL
            WRITE(NW,60)I,DGZERO(I),DGCALC,DGDEVN,
     *      EMF(I),EMFCAL,EMFDEV,TK(I),PO2REF(I),
     *      PO2(I),IFIX(SNGL(BATHTK(I))),PAS406(BATHTK(I))
  200    CONTINUE
C
C CALCULE G FUNCTION FOR THE UNKNOWN SPECIES:
C
         IF(M1.LE.0)GO TO 100
         GA(M)=Q(1)/STOIC(M)
         GB(M)=Q(2)/STOIC(M)
         GC(M)=0.0
         GD(M)=0.0
         GE(M)=0.0
         GF(M)=Q(3)/(2.303D00*STOIC(M))
         GG(M)=0.0
         DO 65 I=1,M1
            GA(M)=GA(M)-STOIC(I)*GA(I)/STOIC(M)
            GB(M)=GB(M)-STOIC(I)*GB(I)/STOIC(M)
            GC(M)=GC(M)-STOIC(I)*GC(I)/STOIC(M)
            GD(M)=GD(M)-STOIC(I)*GD(I)/STOIC(M)
            GE(M)=GE(M)-STOIC(I)*GE(I)/STOIC(M)
            GF(M)=GF(M)-STOIC(I)*GF(I)/STOIC(M)
            GG(M)=GG(M)-STOIC(I)*GG(I)/STOIC(M)
65       CONTINUE
C
C CALCULATE DH298, S298 AND CP FOR THE UNKNOWN SPECIES
C
         CPA(M)=-GF(M)
         CPB(M)=-GC(M)*2.0D00
         CPC(M)=-GG(M)*2.0D00
         CPD(M)=-GD(M)*6.0D00
         DT=298.0D00
         DH298(M)=GA(M)+CPA(M)*DT+CPB(M)*DT**2/2.0D00-CPC(M)/DT
     *           +CPD(M)*DT**3/3.0D00
         S298(M)=-GB(M)+CPA(M)+CPA(M)*DLOG(DT)+CPB(M)*DT
     *          -CPC(M)/(2.0D00*DT**2)+CPD(M)*DT**2/2.0D00
         WRITE(6,80)(SPHASE(M,J),J=1,18),STOIC(M),DH298(M),S298(M)
     *   ,CPA(M),CPB(M),CPC(M),CPD(M)
         WRITE(NW,950)
100    CONTINUE
       WRITE(6,998)
       GO TO 1
C
C FORMATS
C
20     FORMAT(18A4)
30     FORMAT(1H1,1X,18A4)
35     FORMAT(/,' Metal-arsenate = Metal-oxide + I.O2(g) + J.As4O6(g)',
     1 '   I =',F6.2,',  J =',F6.2)
70     FORMAT(///,' DGZERO = a + bT + cT*log10(T)',/
     1,' a =',E16.8,/,' b =',E16.8,/,' c =',E16.8,/
     2,'r.m.s. deviation =',F7.1)
71     FORMAT(/,'      DGZERO  DGCALC    DG(DEVN) EMF EMFCALC EMF(DEVN)'
     * ,'  TK    PO2REF     O2(EXP) BATHTK PAS4O6')
60     FORMAT(1X,I3,2F9.0,F6.1,F7.1,F7.1,F6.1,
     *F10.1,1X,1PE10.3,1PE10.3,I4,1X,1PE10.3)
80     FORMAT(/,1X,18A4,/,' STOICHIOMETRY = ',F6.3,/,
     *' DH(298) = ',E13.6,',   S(298) = ',E13.6,
     */,' CP = CP(A) + CP(B).T + CP(C)/T**2 + CP(D).T**2',
     */,' CP(A) = ',E13.6,', CP(B) = ',E13.6,', CP(C) = ',E13.6,
     *' CP(D) = ',E13.6)
950    FORMAT(' ------------------------------------------------------'
     *,'--------------------------------')
998    FORMAT(////)
999    CONTINUE
       STOP
       END
```

```
C-----------------------------------------------------------------------
C SUBROUTINE SQUARE PERFORMS A LEAST SQUARES ANALYSIS
C
      SUBROUTINE SQUARE(Y,X,MAX,N,M,B,S)
      DIMENSION X(99,3),Y(99),A(3,3),XSUM(3),B(3)
      DOUBLE PRECISION Y,X,B,S,A,XSUM,FN,YSUM,HOLDA,YCALCI, ZERO
      ZERO = 0.0
      DO 3 J=1,M
    3 XSUM(J) = ZERO
      FN = N
      YSUM = ZERO
      DO 4 I=1,N
      YSUM = YSUM + Y(I)
      DO 4 J=1,M
    4 XSUM(J) = XSUM(J) + X(I,J)
      DO 5 I=1,N
      Y(I) = (FN*Y(I) )/YSUM
      DO 5 J=1,M
    5 X(I,J) = (FN*X(I,J) )/XSUM(J)
      DO 30 J=1,M
      B(J) = ZERO
      DO 10 I=1,N
      B(J) = B(J) + X(I,J)*Y(I)
   10 CONTINUE
      DO 30 K=1,M
      A(J,K) = ZERO
      DO 20 I=1,N
      A(J,K) = A(J,K) + X(I,J)*X(I,K)
   20 CONTINUE
   30 CONTINUE
      DO 350 K=1,M
      DO 310 J=1,M
      HOLDA = A(J,K)
      IF (HOLDA .EQ. ZERO ) GO TO 310
  901 DO 300 L=1,M
      IF (A(J,L).EQ. ZERO) GO TO 300
  912 A(J,L) = A(J,L)/HOLDA
  300 CONTINUE
      B(J) = B(J)/HOLDA
  310 CONTINUE
      DO 330 J=1,M
      IF (J.EQ.K) GO TO 330
      IF (A(J,K).EQ. ZERO) GO TO 330
  933 DO 320 L=K,M
  944 A(J,L) = A(J,L) - A(K,L)
  320 CONTINUE
      B(J) = B(J) - B(K)
  330 CONTINUE
  350 CONTINUE
      DO 400 K = 1,M
      B(K) = B(K)/A(K,K)
  400 CONTINUE
      DO 11 I=1,N
      Y(I) = (YSUM*Y(I) )/FN
      DO 11 J=1,M
   11 X(I,J) = (XSUM(J)*X(I,J) )/FN
      DO 12 J=1,M
   12 B(J) = (B(J)*YSUM)/XSUM(J)
      S = 0.0
      DO 600 I=1,N
      YCALCI = 0.0
      DO 500 J=1,M
      YCALCI = YCALCI + B(J)*X(I,J)
  500 CONTINUE
      S = S + (Y(I) - YCALCI)**2
  600 CONTINUE
      RETURN
      END
```

```
C-------------------------------------------------------------------------
      SUBROUTINE GFUNC
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/COM1/$CHAR(10,18),H(10),S(10),A(10),B(10),C(10),D(10)
     *,GA(10),GB(10),GC(10),GD(10),GE(10),GF(10),GG(10),STOIC(10),N
      DO 20 I=1,N
         DT=298.0D00
         GA(I)=H(I)-A(I)*DT-B(I)*DT**2/2.0D00+C(I)/DT-D(I)*DT**3/3.0D00
         GB(I)=A(I)-S(I)+A(I)*DLOG(DT)+B(I)*DT
     *       -C(I)/(2.0D00*DT**2)+D(I)*DT**2/2.0D00
         GC(I)=-B(I)/2.0000
         GD(I)=-D(I)/6.0D00
         GE(I)=0.0D00
         GF(I)=-A(I)
         GG(I)=-C(I)/2.0D00
20    CONTINUE
      RETURN
      END

C-------------------------------------------------------------------------
C SUBROUTINE READER PERMITS A FREE FORMAT READ
C
/INC FORT.READER.PUBL
C
C-------------------------------------------------------------------------
/DATA
/INCLUDE DATA.ARSENIC
*END
```

## ANNEXE B - Sample data stored in DATA.ARSENIC

```
      2ND RUN NOV. 3
*      O2(G)
      -1.25
      0 49.005 7.160 1.0E-3 -0.40E5
      NIO(S)
      1
      -57200.0 9.654 11.180 2.020E-3
      AS4O6(G)
      0.25
      -289000.0 91.0 27.75 5.85E-2 0 3.284E-5
      NIAS(S)
      -1
      0
      -1.25 0.25
      790.8 -731.7 1 460.5
      793.3 -732.6 1 457.6
      791.6 -731.4 1 458.2
      752.8 -746.2 1 456.5
      751.7 -746.2 1 456.6
      714.4 -757.3 1 457.0
      714.8 -757.5 1 456.3
      686.2 -766.5 1 457.8
      771.7 -741.0 1 458.4
      0
```

## ANNEXE C - Thermodynamic data of selected compounds taken from F*A*C*T

FORMULA: O2

NAME: OXYGEN

FORMULA WEIGHT: 31.999

| PHASE | NAME | CP RANGE (K) | COMMENTS |
|---|---|---|---|
| G1 | GAS | 298.0 - 3000.0 | |
| AQ | AQUEOUS | 298.0 - 573.0 | |

CP = A + 1.0E-3*B*T(K) + 1.0E5*C*T(K)**-2 + 1.0E-6*D*T(K)**2

| PHASE | DH(298) (KCAL) | S(298) (CAL/K) | DENSITY (G/CM**3) | A | B | C | D |
|---|---|---|---|---|---|---|---|
| | | | | (CAL/K) | | | |
| G1 | 0.0 | 49.005 | IDEAL | 7.160 | 1.000 | -0.400 | 0.0 |
| AQ | -2.800 | 26.500 | ----- | 38.774 | 7.673 | 7.556 | 0.0 |

FORMULA: NI1O

NAME: NICKEL MONOXIDE

FORMULA WEIGHT: 74.709

| PHASE | NAME | CP RANGE (K) | COMMENTS |
|---|---|---|---|
| S1 | SOLID-A | 298.0 - 525.0 | D H TRANS ( 525.00 K) = 0.010 (KCAL) |
| S2 | SOLID-B | 525.0 - 565.0 | D H TRANS ( 565.00 K) = 0.010 (KCAL) |
| S3 | SOLID-C | 565.0 - 1800.0 | |
| G1 | GAS | 298.0 - 2000.0 | |

CP = A + 1.0E-3*B*T(K) + 1.0E5*C*T(K)**-2 + 1.0E-6*D*T(K)**2

| PHASE | DH(298) (KCAL) | S(298) (CAL/K) | DENSITY (G/CM**3) | A | B | C | D |
|---|---|---|---|---|---|---|---|
| | | | | (CAL/K) | | | |
| S1 | -57.500 | 9.100 | 6.670 | -4.990 | 37.580 | 3.890 | 0.0 |
| S2 | -57.698 | 8.450 | 6.670 | 13.880 | 0.0 | 0.0 | 0.0 |
| S3 | -57.200 | 9.654 | 6.670 | 11.180 | 2.020 | 0.0 | 0.0 |
| G1 | 74.000 | 57.700 | IDEAL | 9.685 | 0.226 | -1.478 | 0.0 |

REFERENCE:

'CONTRIBUTIONS TO THE DATA ON THEORETICAL METALLURGY',
XVI. THERMODYNAMIC PROPERTIES OF NICKEL AND ITS INORGANIC COMPOUNDS,
ALLA D. MAH AND L.B. PANKRATZ,
U.S. BUREAU OF MINES BULLETIN 668, WASHINGTON, 1976.
APPENDED TO:
'THERMOCHEMICAL PROPERTIES OF INORGANIC SUBSTANCES',
I. BARIN, O. KNACKE, AND O. KUBASCHEWSKI,
SPRINGER-VERLAG, BERLIN, 1977.

## ANNEXE D - Results of the sample calculation for the reaction

$$NiAs(s) + 1.25O_2(g) = NiO(s) + 0.25\ As_4O_6(g)$$

```
       2ND RUN NOV. 3

*      O2(G)
STOICHIOMETRY = -1.250
DH(298) =  0.000000D 00,   S(298) =  0.490050D 02
CP = CP(A) + CP(B).T + CP(C)/T**2 + CP(D).T**2
CP(A) =  0.716000D 01, CP(B) =  0.100000D-02, CP(C) = -0.400000D 05 CP(D) =  0.000000D 00

     NIO(S)
STOICHIOMETRY =  1.000
DH(298) = -0.572000D 05,   S(298) =  0.965400D 01
CP = CP(A) + CP(B).T + CP(C)/T**2 + CP(D).T**2
CP(A) =  0.111800D 02, CP(B) =  0.202000D-02, CP(C) =  0.000000D 00 CP(D) =  0.000000D 00

     AS4O6(G)
STOICHIOMETRY =  0.250
DH(298) = -0.289000D 06,   S(298) =  0.910000D 02
CP = CP(A) + CP(B).T + CP(C)/T**2 + CP(D).T**2
CP(A) =  0.277500D 02, CP(B) =  0.585000D-01, CP(C) =  0.000000D 00 CP(D) =  0.328400D-04
-------------------------------------------------------------------------------

Metal-arsenate = Metal-oxide + I.O2(g) + J.As4O6(g)   I = -1.25,  J =  0.25


DGZERO = a + b*T + c*T*log10(T)
a = -0.113779580 06
b =  0.407958230 02
c =  0.000000000 00
r.m.s. deviation =  101.5

    DGZERO   DGCALC    DG(DEVN) EMF EMFCALC EMF(DEVN)   TK    PO2REF      O2(EXP) BATHTK PAS4O6
 1  -81426.  -81518.   92.6 -731.7 -732.5   0.8      790.8  1.000D 00 2.198D-19 460  5.373D-04
 2  -81444.  -81416. -28.0 -732.6 -732.4  -0.2      793.3  1.000D 00 2.387D-19 457  4.433D-04
 3  -81328.  -81486.  157.5 -731.4 -732.8   1.4     791.6  1.000D 00 2.336D-19 458  4.614D-04
 4  -83141.  -83068. -72.1 -746.2 -745.6  -0.6      752.8  1.000D 00 1.027D-20 456  4.119D-04
 5  -83147.  -83113. -33.9 -746.2 -745.9  -0.3      751.7  1.000D 00 9.604D-21 456  4.146D-04
 6  -84581.  -84635.   53.8 -757.3 -757.8   0.5     714.4  1.000D 00 4.207D-22 457  4.259D-04
 7  -84586.  -84619.   32.6 -757.5 -757.8   0.3     714.8  1.000D 00 4.269D-22 456  4.064D-04
 8  -85769.  -85785.   16.3 -766.5 -766.6   0.1     686.2  1.000D 00 2.987D-23 457  4.492D-04
 9  -82516.  -82297.-218.9 -741.0 -739.1  -1.9      771.7  1.000D 00 4.336D-20 458  4.676D-04

     NIAS(S)
STOICHIOMETRY = -1.000
DH(298) = -0.156704D 05,   S(298) =  0.119436D 02
CP = CP(A) + CP(B).T + CP(C)/T**2 + CP(D).T**2
CP(A) =  0.916750D 01, CP(B) =  0.153950D-01, CP(C) =  0.500000D 05 CP(D) =  0.821000D-05
-------------------------------------------------------------------------------
```

DGZERO = a + b*T + c*T*log10(T)
a = -0.68781387D 05
b = -0.42031673D 03
c = 0.13948904D 03
r.m.s. deviation = 91.1

| | DGZERO | DGCALC | DG(DEVN) | EMF | EMFCALC | EMF(DEVN) | TK | PO2REF | O2(EXP) | BATHTK | PAS406 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -81426. | -81488. | 62.5 | -731.7 | -732.2 | 0.5 | 790.8 | 1.000D 00 | 2.198D-19 | 460 | 5.373D-04 |
| 2 | -81444. | -81377. | -67.7 | -732.6 | -732.0 | -0.6 | 793.3 | 1.000D 00 | 2.387D-19 | 457 | 4.433D-04 |
| 3 | -81328. | -81452. | 124.3 | -731.4 | -732.5 | 1.1 | 791.6 | 1.000D 00 | 2.336D-19 | 458 | 4.614D-04 |
| 4 | -83141. | -83123. | -17.2 | -746.2 | -746.1 | -0.1 | 752.8 | 1.000D 00 | 1.027D-20 | 456 | 4.119D-04 |
| 5 | -83147. | -83169. | 21.6 | -746.2 | -746.4 | 0.2 | 751.7 | 1.000D 00 | 9.604D-21 | 456 | 4.146D-04 |
| 6 | -84581. | -84658. | 76.4 | -757.3 | -758.0 | 0.7 | 714.4 | 1.000D 00 | 4.207D-22 | 457 | 4.259D-04 |
| 7 | -84586. | -84642. | 56.2 | -757.5 | -758.0 | 0.5 | 714.8 | 1.000D 00 | 4.269D-22 | 456 | 4.064D-04 |
| 8 | -85769. | -85705. | -64.1 | -766.5 | -765.9 | -0.6 | 686.2 | 1.000D 00 | 2.987D-23 | 457 | 4.492D-04 |
| 9 | -82516. | -82324. | -192.1 | -741.0 | -739.3 | -1.7 | 771.7 | 1.000D 00 | 4.336D-20 | 458 | 4.676D-04 |

NIAS(S)
STOICHIOMETRY = -1.000
DH(298) = -0.426192D 05, S(298) = -0.435366D 02
CP = CP(A) + CP(B).T + CP(C)/T**2 + CP(D).T**2
CP(A) = 0.697359D 02, CP(B) = 0.153950D-01, CP(C) = 0.500000D 05 CP(D) = 0.821000D-05

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POOR

QUALITY

ORIGINAL